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ACADEMIC SEGMENT OF UKRAINIAN GRID INFRASTRUCTURE

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Ukrainian Academic Grid (UAG) is presented as a powerful computing resource for fundamental and applied scientific research which are carried out at the NAS of Ukraine (NASU). Information on activity, structure, computational power and problems of UAG follows a short historical outlook. Contribution of UAG to the Ukrainian National Grid Initiative (UNGI) is emphasized. Examples of a cooperation of NASU institutes with international grid projects and organizations, in particular, with WLCG, EGEE and EGI are presented. Prospects of UAG and UNGI activities in developing various Grid applications within various scientific areas are shown.

INTRODUCTION

An area of information-computing technologies has been fundamentally modified afterwards the basic idea of the spatially distributed computing appeared in the eighties of the last century. Grid technologies occupied an important unless the most quickly progressing place in this area. Their principles have been logically and adequately formulated by I. Foster and C. Kesselman [1]. It is the authors's opinion that "*A computational grid is a hardware and software infrastructure that provides dependable, consistent, pervasive, and inexpensive access to high-end computational capabilities*". In other words the grid looks to users like one powerful computer with unlimited resources (processors, RAM, storages etc.).

The impetuous development of grid technologies in the world is caused by the increasing complexity of computational problems in the various human activities, on the one hand, and by the fast progress of computer material resources and the perfect element resources of modern computers, on the other one. An increase of the computing capacity and the Internet links getting cheaper rate play almost a key role in this process inasmuch as grid uses the Internet as data communications medium.

From the outset grid technologies have been mainly applied for high energy physics. Now they have already penetrated in the various fundamental and applied sciences (from physics and astrophysics till Earth sciences and biomedical ones) and are steadily advancing in industry, economics and social life. It is timely to refer to the analysis done by the INSIGHT Research Corporation in 2006 [2]. According to published thesis "Grid Computing: A Vertical Market Perspective 2006-2011" the investment to the Grid technologies will increase from 1.84 billion in 2006 to 24.52 billion in 2011 (fig. 1).

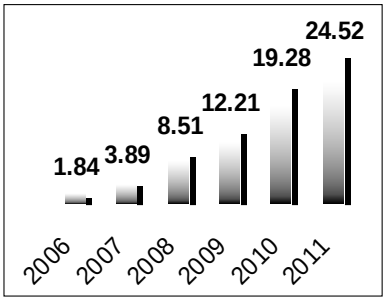

Fig. 1. Funds for developing Grid in the world (in billion dollars)

Developing the grid technologies, building the national and international grid infrastructures is naturally fitting in the objective globalization processes in economics, sciences and culture. The international associations and projects are playing now an increasingly appreciable role in sciences and economics. Moreover, it is a challenge for any country to realize independently some research projects such as program of studying a microcosm using the most powerful collider of elementary particles and nuclei — LHC (Large Hadron Collider) at CERN. These projects require quite serious data-processing support which grid can satisfy.

Nowadays there is none of highly developed countries which reject an idea to build up a proper grid network. We can state with assurance a country that has not grid infrastructure and is not drawn into the world Grid community could not even pretend to be a developed one. Thus, a development and application of Grid technologies for the daily social life becomes a strategic trend for each state which is anxious about scientific, economic and social progress.

GRID TECHNOLOGIES AND GRID INFRASTRUCTURE

From the practical view point the grid is a service for sharing spatially distributed computer systems into one vast computing resource to provide more efficient use of computing resources available and to solve the problems which need the serious computing power. Functionally the grid infrastructure has to ensure:

- **Effective intercommunication of heterogeneous computers or computer systems.**
- **HPC — high-performance computing**. Grid allows to share resources for performing great computations (for example, data processing from LHC at CERN), which cannot be done using an individual computer system.
- **Processing of huge data array**, which can be stored in different remote memory. These calculations must usually occur with extra load conditions in computing and communication resources.
- **Support and operational compatibility of different virtual organizations (VOs).** Grid has to support a cooperative activity of the real VOs members and to provide, as required, the intercommunication of different VOs through the middleware.

To realize the functions listed above grid as a data processing infrastructure must have three principal components:

1) clusters or single computers (proper computing and operating resources);
2) Internet high-speed channels, (Internet HSC);
3) middleware.

The necessity to use the grid technologies in the National Academy of Sciences of Ukraine (NASU) mainly evolves from recent research areas, appearance of new computational problems with unexampled high demands to computation and data processing capacity, computation speed as well. These problems arise, for example, in high energy physics and astrophysics, biophysics and biology, science of materials, Earth sciences and many others, both fundamental and applied studies. As it was proved grid technologies can be installed (with minimal financial costs) into a daily practice of institute regardless of its geographical lo-

cation in such a way that any researcher gains the access to the computational resources even though his institute does not have such resources.

The factors listed above have been counted for working up the academic grid project. The particular qualities and characteristics of grid technologies as well as the building of grid systems utilizing an experience of other countries and numerous grid projects have been taken into account. The efforts were made to avoid the subsequent difficulties encountered in building the branched grid infrastructure of NASU and on the whole in Ukraine. First of all, it concerns the limited funding which forces to formulate a certain strategy and tactics; secondly, the deficiency of qualified specialists which know about the grid technologies (in particular, among the specialists who does not work with the information discipline).

HISTORY OF GRID INFRASTRUCTURE CREATION IN NASU

The chronology of facts and events related to the creation of the first Ukrainian grid infrastructure clearly demonstrates how these problems were overcome by the initiators of grid infrastructure realization in Ukraine.

While computational clusters were created since 1999 (Glushkov Institute of Cibernetics, NASU (Kiev), Kiev National University, Institute of Condensed Systems, NASU (Lviv), State Scientific Institution "Monocristal", NASU (Kharkiv) the first grid site appeared in Ukraine at 2004. It was created by the group of physicists from National Scientific Center "Kharkov Institute of Physics and Technology". The computer cluster was built in the framework of collaboration with Joint Institute of Nuclear Researches (JINR, Dubna, Russia) and participation in CMS (Compact Muon Solenoid) experiment at LHC which is one of the large experiments planned to run at CERN (Geneva, Switzerland).

The practical steps in realization of more or less systematic approach creating grid system in the country were made at 2005 only.

During several last years the scientists of the Bogolyubov Institute for Theoretical Physics of NASU were discussing the problems of constructing the powerful computing capacities necessary for an analysis of experimental data in high energy physics at the Ukrainian academic Institutes and Universities. Eventually at the end of 2005 the consensus has been reached that the Ukrainian community will try to contribute at CERN not only to physics but to the computing support of the future LHC experiments. Such a collaboration will provide, first of all, a direct access to the new data necessary for the theorists to develop and verify new physical ideas and, secondly, will help to the Ukrainian physicists "to be in the centre of events" due to the grid possibilities maintaining the close professional contacts with CERN which is a world leading research organization.

It has been underlined that the grid technology application is an extremely advanced method not only for high energy physics, but it can help to solve various fundamental and practical high computational problems in many branches of fundamental research. It opens the new horizons in the research process as well and activates the international cooperation in different human activities. That was a strong motivation for the initiators to be targeted on creating the grid infrastructure which could be used by the NASU scientists and specialists from other institutions operating with high computational problems.

The conception of grid development and its application in BITP has been unambiguously supported by the director of Institute, Academician A. Zagorodny. At that time there was not high speed channel in the Institute for Theoretical Physics and the prototype grid site of 2 servers has been created in Computer Center of Taras Shevchenko Kiev National University (CC KNU). Due to a tight collaboration of BITP and ALICE Collaboration (A Large Ion Collider Experiment) [3] the grid site has been certified by AliEn-grid (ALICE-Enviroment-grid) [4] (the Grid organization for providing the computing resource for the ALICE experiment at CERN).

In June 2005 the session of Coordinating Board for Informatics of NASU was held at BITP. The project to create the grid computer cluster at BITP has been comprehensively discussed and approved. The practical work was trigged up with quite clear prospects. At the end of 2005 the computer cluster of 10 nods (double processors) has been built and the grid middleware has been installed.

Several events which took place on April 2006 have provided the progress in the grid development at BITP and NASU. The Institute received the fiber-optic channel with capacity 2 Mb/s and an access to the academic Internet network – UARNET. The first grid tasks which had come to the cluster from CERN and the other AliEn-grid Institutes were quickly elaborated.

On April 25 the National Academy of Sciences of Ukraine has been officially affiliated to the WLCG (Worldwide LHC Computing Grid [5]) organization which has to coordinate the computer (Grid) support for LHC experiments. By April 2006 Conception of the Grid infrastructure development in Ukraine has been approved by the NASU Presidium. At the end of 2006 new grid clusters have been built in five institutes of NASU and in December the first prototype grid system of 2 clusters (BITP and KNU) has been put into operation to process grid network using NorduGrid middleware. Basing on this gained experience it became possible already in April 2007 to combine clusters of six NASU Institutes into the first Ukrainian grid segment.

According to the Program "Grid technologies development and clustering in NASU" it was proposed to solve the main tasks of the Program in 3 phases:

First phase: clustering, pushing forward a collaboration of the Ukrainian scientists in the LHC projects at CERN, propagating an idea of the NASU official participation in WLCG.

Second phase: creation of the first grid segment at NASU and increasing a number of clusters.

Third phase: establishing the Ukrainian Academic Grid (UAG) and presenting UAG as a coordinating center, providing an official participation of NASU in the international (especially European) Grid organizations and projects, continuing the cluster creation.

Tasks of these three phases are practically realized up to now. Ukrainian Academic Grid is successfully functioning.

UKRAINIAN ACADEMIC GRID

Ukrainian Academic Grid (UAG) is a grid infrastructure to share the computer resources of the NASU institutes and universities as well.

The principal tasks of the UAG is to develop the distributed computings and grid technologies to advance computationally intensive fundamental and applied studies NASU. Besides, UAG has to ensure a participation of the Ukrainian scientists in various topical international grid projects.

Structure and organizational management of the UAG

It is well known that grid system is based on three principal elements: computer resources (clusters), high-speed and reliable access of resources to Internet and middleware which unifies these resources into one computer system.

Though the middleware was available even at the beginning of the grid infrastructure creation the clusters and fiber-optic network of NASU were simultaneously built with the grid facilities system development.

The well-known Beowulf idea (www.beowulf.org) as a conceptual model for the computer cluster construction was selected and adopted for realization in NASU. This conception is based on using servers with standard PC architecture, distributed main storage and Gigabit Ethernet technology which unifies computer system. So, all Grid clusters in NASU are built with x86, x86_64 architecture, two- (four-) processor servers of 1-4 GB main storage and 36-500 GB HDD. To provide the inter-server exchange 1GB/s switchers have been used and only in some clusters the InfiniBand is exploited.

At present the UAG shares resources (more than 2500 CPU and about 300 TB of disk memory) of the next organizations (fig. 2).

It should be emphasized that the footprint on hard disks of computer nodes is used for operating system (loading from local disks), program packages and temporary files but it is inaccessible to store the user's files. Each cluster has its disk array to store programs, user's data and information of common use. A free distributed operational system Linux of various modifications (Scientific Linux 2.6.9, Fedora 2.6, CentOS-4.6) on clusters is installed and the task management system OpenPBS is used to start tasks and allocate the cluster utilization.

The idea to enlarge the grid infrastructure user base via the so-called access grid platforms, i.e. the grid clusters with "minimal configuration", has been conceived realizing the NASU Program. Such a cluster holds the control server with installed middleware and minimal computing resource. Working permanently in the conditions of limited funding a system of the access grid platforms proposed and developed in the NASU grid infrastructure allows the specialists of Institutes where there is no an operable cluster to use the academic grid full profile. A local resource broker using available network resources distributes the tasks among the grid infrastructure clusters as the computing requests (small problems require a hands-on operation and large-scale ones are directed to more powerful clusters). With the funds available any mini cluster can be easily is easily extended to the full scale cluster. This policy makes it possible to train system administrators for the work with more power clusters.

The high-speed and reliable access channel to Internet networking is one of the necessary conditions at the grid infrastructure building. Ukrainian Academic and Research Network (UARNET) has built the infrastructure which is capable to unify the academic institutions with fiber-optic channels (capacity 100 Mb/s).

In the Institute for Theoretical Physics which is responsible for the academic grid program running the UAG web site (http://uag.bitp.grid.ua) has been designed whereat the information on Grid technologies and Grid development over the world, news and publications can be found.

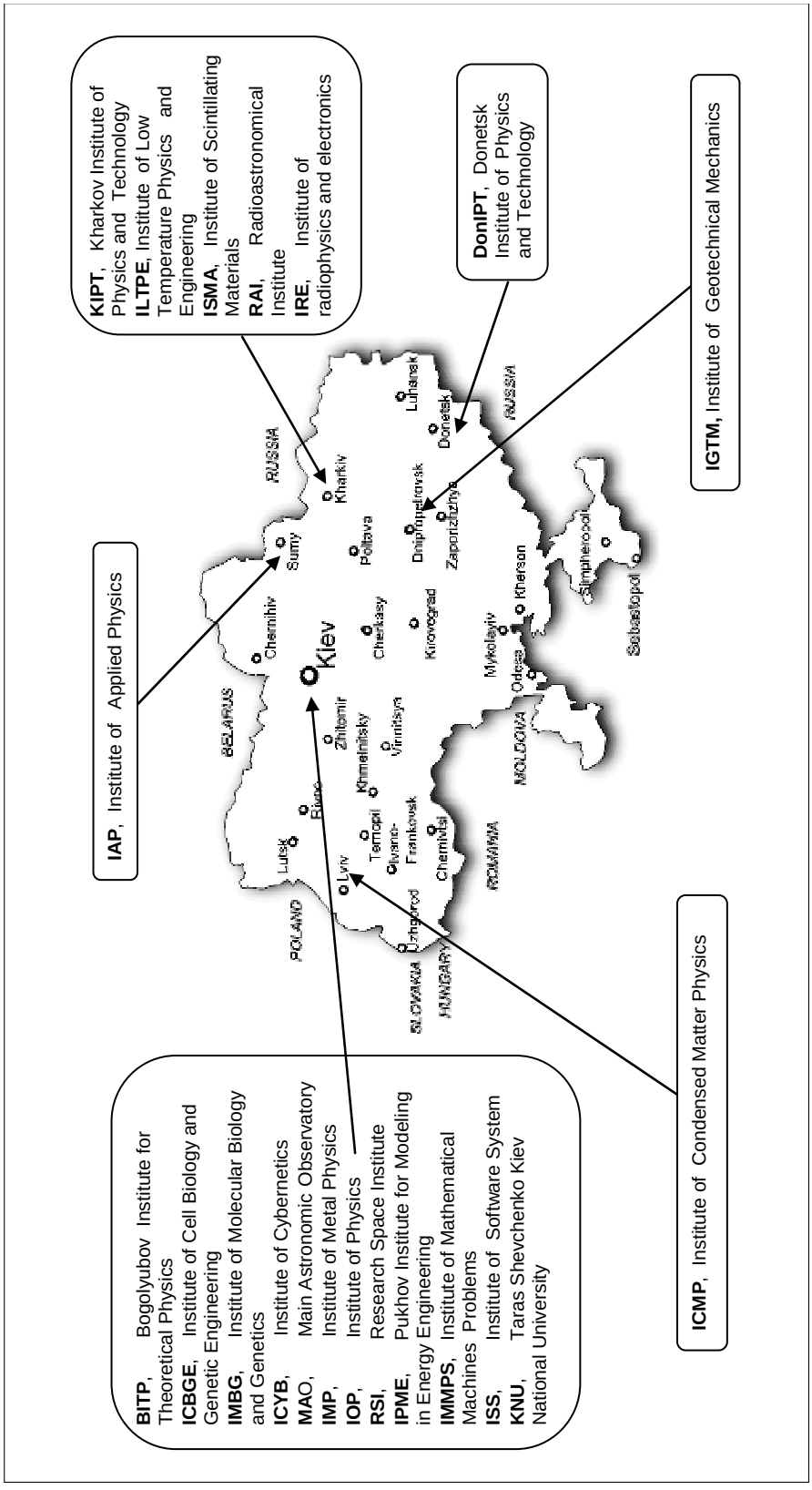

Fig. 2. Ukrainian Academic Grid

Today UAG is operating under the ARC NorduGrid middleware. However in the European Grid projects (WLCG, EGEE [6], EGI [7]) the gLite middleware is recommended as one the key elements. Then it is clear the task to install gLite instead (or in parallel) of ARC middleware in the NASU Grid infrastructure becomes a work of the first priority.

To solve the "**Interoperability**" and "**Interoperate**" problems the software product GridWay [8] has been chosen as an adapter. More details about this activity in UAG are given in the [9,10].

Fundamental and applied tasks to be solved in UAG

First of all, we consider the NASU grid infrastructure both as a supporting equipment for solving the fundamental and applied problems and as a ground wherein the grid technology methods are proved in accomplishment of various tasks. These methods could and should be used then in the national grid infrastructure whose the function is far wider than the research data computing. Nevertheless, below it is an appropriate list of the scientific areas where new UAG facilities have been already used.

High energy physics

LHC (CERN) experimental data processing, their analysis and comparison to the theoretical results and phenomenological models aiming the full scale participation of the Ukrainian institutes in the ALICE experiments (BITP, KNU, IC, KIPT, ISMA, NTU KPI) and CMS ones (KIPT).

Astrophysics and astronomy

- Dynamical computing of an evolution of the star concentration in the Galaxy external field. The hydrodynamic modeling of collision and fragmentation of the molecular clouds. Analysis of N-body algorithm and parallel computing on the GRAPE clusters. Cooperation with AstroGrid-D (MAO).
- Theoretical analysis and the observation processing of primary, roentgen and gamma radiation data which are obtained from the satellite telescopes INTEGRAL, SWIFT and others (BITP, KNU, MAO).
- Creation and formation of VIRGO – VIRtual Gamma and Roentgen Observatory (BITP, KNU).
- Development of nuclei activity models of Galaxy and star concentrations. Testing the dark matter and dark energy models. Collaboration with Lausanne and Geneva universities (BITP, GAO).

Biophysics and biology

- Computing of thermodynamic characteristics, infrared and electron spectra of sputter DNA fragments. Study of bionanohybrid system structures composed by DNA and RNA of different sequence (ILTPE, IC).
- Molecular dynamic computing of Fts-Z-protein systems with the low-molecular associations (ICBGE).
- Computer simulation of the spatial structure and molecular dynamics of cytokine-tyrosine-RNA synthetase (IMBG).

Nanotechnologies

- Computing of nanostructure oxides which seem to be perspective high-temperature superconductors, as well as physical characteristics of the DNA fragment with transition metal ions which could be good nano-conductors.

- Computing of structures and interaction energy of bio-nano-hybrids on basis of the single-shell carbon nano-tubes with the various bio-objects (ILTPE, IMP, IC).

Environment monitoring

- Weather forecast parameters on the Ukrainian terrain based on the computer simulation and satellite data. Estimate of biodiversity as ecologic parameter on Ukrainian terrain (ISR, IC).
- Development of GEO-UA information infrastructure (ISR).

Structuring UAG

The future development of grid technologies in NASU should be focused on their application in the specific research. There are three directions for creating and using the grid technologies which have to be applied in the daily research work in the near future:

- work out new packages for computing on one multiprocessor cluster and on several various distributed clusters as well;
- adapt the relevant middleware for parallel processing;
- use the developed and free distributed license middleware which has been already tested in domestic and foreign institutions.

It is well-known fact there are a lot of highly-qualified specialists in Ukraine and in NASU, in particular, which are able to resolve the problems of this type. There is a need to manage and provide them with the financial and material resources as well as the cooperation between the computer specialists and physicists, chemists, biologists, engineers and others who are interested in the Grid applications and feel this cooperation will be fruitful.

The strategic emphasis in development of UAG should be primarily placed on the creation of such a system which is based on the power supercomputer centres allowing the distributed parallel computing with using ten or even hundred processors. Then any academic institution in Ukraine or research group could have a required time for computing and the facilities of these centers could be optimally used with the grid technology advantages. The world experience, in particular, demonstrates a prospect of such an approach. At the same time there is a need to increase a quantity of the grid sites in the NASU institutes in order to more and more scientists could have an access to the large computing resources.

It is essential to realize that the grid infrastructure with a lot of grid sites can not be merely global computational resources with minimal management. At 2009 UAG has 22 powerful grid clusters and the access grid network platforms. In the world practice examples the grid infrastructure organizations abound within the big projects which consolidate the institutes and laboratories of many countries as well as within the national projects for the countries working separately.

According to the WLCG scheme the infrastructure of UAG should be built as three-level system in respect to an **organization and management**:

First level: Basic Coordinating Centre (BCC) which governs UAG mainly through the regional centres.

Second level: Regional Operating Centres (ROC) which coordinate the activity of grid sites (a Grid site (GS) is a grid cluster or an access platform) in regions.

Third level: Separate grid sites (institutes) or minimal grid network access platforms which belong, as a rule, to any virtual organization (VO). VO temporarily joins institutes (not necessarily from the same region) of common scientific interests to solve a problem.

This is ensured that due to the large performance of grid infrastructure optimized, its stability and reliability are controlled, and the workload of some of its elements is governed. Basic coordination center of NASU consists of teams which provide such a performance.

As to the **grid technology application** for solving various research problems and tasks UAG has to unify the special virtual organizations which can be both permanent and temporary as well as to enter large international unions and projects.

The principal BCC teams and their functions are as follows.

Research and analytical team is to work out and to confirm the BCC activity, research projects on grid technology application in the different fields, to analyze perspective trends of research in the grid technologies and their realization, to make the expert evaluation of new propositions and projects for development and the grid technology applications.

Team of international contacts. The key task of this team is in the development of cooperation with the international organizations and the grid projects in the international collaboration of the UAG participants. The representatives of Regional Operating Centers (ROCs) and Resource Centers of Virtual Organizations (RCVOs) are getting to draw up a plan of the team.

Maintenance team. The team has to assist to the administrators of computer clusters in an installation of system-wide software and to provide computer security, as well as to maitain the working grid nodes. The team coordinator maintains the permanent contact with corresponding specialists of ROC and RCVO, the system administrators and security administrators of each local grid site.

Software support team is to assist administrators of computer clusters in installation of middleware on new clusters and to support the regular and qualitative link with all grid nodes. Moreover, the team experts are responsible for task analysis of the whole grid system, new middleware installation, and compatibility of application software with middleware as well. The team has to know all the answers to any problems appearing in the grid network of NASU.

User support team. Each ROC and grid site must have a portal which should be allocated to the practical directives teaching how anyone might be involved in the Ukranian grid activity and how the process of getting a certificate for virtual organization or grid node, or individual user could be realized. Each user can send a test task to be solved and obtain results using web-site. Web-site has to contain the information concerning the structure of national grid, Internet references to the grid activity documentations and web-sites of each grid site of the national grid as well as reference sources on principal facilities of grid technologies, international grid projects and virtual organizations, announcements on the grid seminars and conferences.

Educating and training centre is to organize the educational process on theoretical and practical basis of the grid technology applications. Virtual educational grid is created on the basis of the display classrooms, the existing and future centers should be timely equipped. The individual education programs to ROC and RCVO administrators, system administrators of Grid clusters and users

should be worked out. Development of educational programs, seminars and organization of continual education should be fulfilled by the experts of KNU and KPI.

The structure of Regional Operating Centres is a similar but the centers are empowered by a less number of functions.

Cooperation with Ukrainian Institutes behind NASU

At the very beginning the NASU researchers are working in full cooperation with the Universities and Institutes behind the NASU structure. Today Higher Schools of the Ministry of Education and Sciences have the good possibilities to teach the IT-specialists, some of them possess the considerable computational resources. They can and must make an essential contribution to the Grid technology development in Ukraine and creation of national wide branched Grid infrastructure.

Scientific and technological project "Creation of National Grid Infrastructure for Research Support" is fulfilling today in Ukraine along with grid project of NASU (BITP is a basic organization with 20 participants). This project was approved by the Ministry of Education and Sciences (MES) to be accomplished in 2007-2008 as a part of the State Program "Information and Communication Technologies in Education and Science". The program provides the formation of the national Grid infrastructure, the creation of Certificate Centre, the maintenance of Ukrainian international data center. NTU KPI is a leading organization in this project and 7 universities and institutions of MES are the contracting parties. It should be mentioned that NASU becomes the contracting party as well.

Taking into account that both projects have similar purposes the MES and NASU started to collaborate. BITP and NTU KPI made an agreement to create the Ukrainian Grid Association which, in accordance to the EGI recommendations, was termed as Ukrainian National Grid Initiative (UNGI). The structure of UNGI was strictly outlined and documented, the immediate and advanced plans which should be realized after accepting and approval the State Program were discussed and fixed. The formal procedure of association registration is very close to be completed now.

It should be emphasized that the active work is now underway on the grid technologies application in the medical institutions. The program of collaboration between the NASU and Academy of Medical Sciences of Ukraine and some big medical centers is successfully working. The NASU is ready to aid and to grant the computational resources for using the gggrid technologies in medical practice in the framework of pilot projects.

International cooperation of UAG

Grid may be considered as a new reinforced instrument for scientific and technological international cooperation. Grid becomes one of the principal factors and locomotives of the globalization process. Science has always an international nature but at the end of previous century because of the fight with the background of economic globalization the proper attention to developing the cooperation principles in the science management was not given in necessary extent. Nevertheless, due to Internet and new scientific projects (for example, Space exploration, the largest colliders in CERN and USA, European project of thermonuclear reactor ITER etc.) the tasks of world science integration have been brought to the fore-

front. New international project called the World Grid could be realized by creating the national and big international grid projects (WLCG, EGEE, GLORIAD, TERAGRID and others). Realizing a stable character of unification tendency and availability of this process in the country the organizers of UAG pay the special efforts to the integration and consolidation of the Ukrainian Grid into the international grid community.

Today the Ukrainian experts are ready to learn the great experience their foreign colleagues, however, they have a lot of achievements as well which could be very practical for the international community of the Grid users. Below we list new trends and activities which as we believe are the quite promising for future cooperation and will provide both sides with a steady progress of the grid technologies.

Ukraine was registered as a non-contracting participant in the EGEE project in 2007. It was planned that the Ukrainian specialists should work out the subject of grid applications (e.g. in high energy physics, astrophysics, life science, earth science) and focus their efforts on education and knowledge propagation of grid and distribution of the grid technologies into medicine and industry.

In May 2007 Ukraine signed Memorandum of Understanding about the participation in EGI. The spectrum of tasks which are of interest for the Ukrainian experts corresponds quite well to the activity which was declared in EGEE.

Starting on April 2006 NASU is a member of the WLCG collaboration. Several academic institutes put their computational resources for common work in WLCG. The researchers of BITP and KIPT accomplish the theoretical and phenomenological tasks together with the technical preparations for the future work in the LHC experiments.

The researchers of the Institute of Space Researches of NASU and of National Space Agency of Ukraine (NSAU) in cooperation with their Chinese colleagues are fruitfully developing and use the grid technologies in the satellite monitoring of Earth surface and water.

The agreement about the joint investigations and cluster computing with GRAPE-cards in the framework of German AstroGrid-D project has been signed by MAO. In the Institutes of biological investigations the negotiations with colleagues of the Western countries about the common projects within the specific VOs are carrying on.

There are no doubts that the international relations of UAG, its collaboration in the grid projects with experts of many countries will be considerably extended and intensified.

PROBLEMS IN UAG

Creating the UAG basic infrastructure we gained the practical experience both in development of clusters and in management of cooperation between the various NASU institutes in the Grid activity. Now we understand better what should be done to guarantee an appreciable progress of computing constituent not only in NASU but in Ukraine, too.

At the same time we met some problems which limit the grid technology distribution, for example:

1. **Lack of information on new computational technologies in the scientific community.** Institutions of informatics should focus more attention on extending the knowledge about these technologies in all academic sub-divisions.

2. **Shortage of the qualified personnel.** First, it occurs that the local networks (if they are present) and primary output to Internet in the NASU Institutes are mainly maintained by the enthusiasts who are the researchers, but not computer specialists. Secondly, even if there is a qualified system administrator in an Institute (usually a young scientist without scientific degree) his salary is very scanty because of the academic regulations of the labour remuneration.

3. **Scarcity of the IT specialists** which understand properly the principles of grid technologies. The world tendency demonstrates the widespread adoption of grid in various human activities, and so there is an urgent need to train students of the computer science.

4. **Lack of high speed Internet links** in many institutes of NASU (in non-academic institutions, especially in regional ones). With a channel capacity growth the traffic cost rapidly increases and so there are no adequate financing in the Institutes to provide the channel capacity required by grid.

SUMMARY

Despite all difficulties and problems in developing of grid technologies in NASU the background of the widest application of grid technologies in Ukraine has been provided. There is a good reason to believe that grid exists and operates in Ukraine, the collaboration with international grid community is intensified and Ukrainian National Grid will be built with joint efforts and occupy a fitting place in the world grid infrastructure.

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